GRATINGS: THEORY AND NUMERIC APPLICATIONS

Tryfon Antonakakis
Fadi Baïda
Abderrahmane Belkhir
Kirill Cherednichenko
Shane Cooper
Richard Craster
Guillaume Demesy
John DeSanto
Gérard Granet
Boris Gralak
Sébastien Guenneau
Daniel Maystre
André Nicolet
Brian Stout
Fréderic Zolla
Benjamin Vial

Evgeny Popov, Editor

Institut Fresnel, Université d'Aix-Marseille, Marseille, France
Femto, Université de Franche-Compté, Besançon, France
Institut Pascal, Université Blaise Pascal, Clermont-Ferrand, France
Colorado School of Mines, Golden, USA
CERN, Geneva, Switzerland
Imperial College London, UK
Cardiff University, Cardiff, UK
Université Mouloud Mammeri, Tizi-Ouzou, Algeria

ISBN: 2-85399-860-4
www.fresnel.fr/numerical-grating-book

ISBN: 2-85399-860-4

First Edition, 2012, Presses universitaires de Provence (PUP)

World Wide Web:

www.fresnel.fr/numerical-grating-book

Institut Fresnel, Université d'Aix-Marseille, CNRS
Faculté Saint Jérôme,
13397 Marseille Cedex 20,
France

Gratings: Theory and Numeric Applications, Evgeny Popov, editor (Institut Fresnel, CNRS, AMU, 2012)

Copyright © 2012 by Institut Fresnel, CNRS, Université d'Aix-Marseille, All Rights Reserved

Editorial Preface

A typical question that almost all of us (the authors' team and other colleagues) has been asked not only once has in general the meaning (although usually being shorter): "What is the best method for modeling of light diffraction by periodic structures?" Unfortunately for the grating codes users, and quite fortunately for the theoreticians and code developers, the answer is quite short, there is no such a bird like the best method.

In the more than 30 years active studies on the subject, I have worked on the theory and numerical applications of several approximate methods, like Rayleigh expansion, coupled-wave theory, beam propagation method, first-order approximations, singular Green's function approximation, effective index medium theory, etc. My conviction is that they are quite useful (otherwise why to exist) for physical understanding, but my heart lies in what is considered as rigorous grating theories. Name 'rigorous' is used in the sense that in establishing the theories, exact vector macroscopic Maxwell equations and boundary conditions are applied without approximations. The approaches become approximate after computer implementation, due to the impossibility to work with infinite number of equations and unknowns, and due to the finite length of the computer word.

Of course, there are always initial approximations and assumptions, like the infinite dimensions of the grating plane, linearity of the optical response, etc. From physical point of view, the main feature of the methods, presented in this book are characterized by the use of optical parameters of different substances as something given by other physical optics theories and the experiment as an ultimate judge.

The necessity to use more than a single rigorous method comes from practice: different optogeometrical structures made of different materials and working in different spectral regions require a variety of methods, because each one is more effective in some cases, and less effective (or failing completely) in others. In addition, each approach is a subject of constant research and development. Grating modeling, grating manufacturing and grating use go hand in hand, and practice provides strong stimuli for the theory development. Vice versa, recent grating technologies and application cannot advance without proper theoretical and numerical support.

When I started my grating studies, the method of coordinate transformations that uses eigenvector technique to integrate the Maxwell equations (sometimes known as the C-method) has just been formulated. It worked perfectly for holographic grating whatever the polarization and the grating material, but failed completely for grooves with steep facets. It took more than 15 years to refine its formulation, so that now it can deal with echelles and pyramidal bumps (in the case of two-dimensional periodicity) with slopes up to 87 deg steepness. However, the method is not at all adapted to lamellar gratings. On the other hand, the Fourier modal method (also known as Rigorous coupled-wave approach, RCW) is perfect for such profiles, but its use in the case of arbitrary grating profiles (e.g., sinusoidal or triangular profiles) in case of metallic grating material causes problems when using a staircase approximation of the profile. The differential method does not use this approximation and could deal with arbitrary profiles, but it took more than 20 years to make it working with metallic gratings in TM (p, or S) polarization. And quite ironically, the improvement came from advances in the competing RCW approach.

These methods are relatively easy for programing nowadays, after solving the numerical problems due to growing exponentials and factorization rules of the product of permittivity and electric field, however there are still some persisting problems for highly conduction metals. In addition, neither the differential, nor the Fourier modal methods can deal with infinitely conducting gratings.

Several methods are quite flexible concerning the geometry of the diffracting objects and the grating material. For example, the integral method can treat inverted profiles, rod gratings with arbitrary cross section, finitely or infinitely conducting materials in any polarization, but its programming require deep mathematical understanding of the singularities and integrability of the Green's functions. Other two flexible methods are quite famous and widely used, even in the form of commercially available codes. These are the finite-element method, and the finite-difference time domain method. The flexibility with respect to the geometrical structure, optical index inhomogeneity and anisotropy, etc. has to be paid by the necessity of sophisticated meshing algorithms and very large sparse matrix manipulations.

These few examples represent only the top of the iceberg, and are invoked to illustrate the basic idea that *the best method has not been invented, yet*. Probably never.

We have tried to gather a team of specialists in rigorous theories of gratings in order to cover as large variety of methods and applications as practically possible. The last such effort dates quite long ago, and it has resulted in the famous *Electromagnetic Theory of Gratings* (ed. R. Petit, Springer, 1980), a book that has long served the community of researchers and optical engineers, but that is now out of press and requires a lot of update and upgrade, something that we hope to achieve, at least partially with this new book.

Our choice of electronic publishing is determined by the desire to ensure larger free access that is not easily available through printed editions. I want to thank all the contributors to this Edition. Special thanks are due to my colleagues Fréderic Forestier and Boris Gralak for the technical efforts to make the electronic publishing possible.

Marseille, France Evgeny Popov
December 2012

Table of Contents with Web and Bibliographic Records:

www.fresnel.fr/files/gratings/GratingsTheoryandNumericApplications.pdf

1. E. Popov, "Introduction to Diffraction Gratings: Summary of Applications," ch.1 of *Gratings: Theory and Numeric Applications*, ed. E. Popov (Institut Fresnel, CNRS, AMU, 2012) 3
www.fresnel.fr/files/gratings/Chapter1.pdf

2. D. Maystre, "Analytic Properties of Diffraction Gratings," ch.2 of *Gratings: Theory and Numeric Applications*, ed. E. Popov (Institut Fresnel, CNRS, AMU, 2012) 29
www.fresnel.fr/files/gratings/Chapter2.pdf

3. J. DeSanto, "Spectral Methods for Gratings," ch.3 of *Gratings: Theory and Numeric Applications*, ed. E. Popov (Institut Fresnel, CNRS, AMU, 2012) 55
www.fresnel.fr/files/gratings/Chapter3.pdf

4. D. Maystre and E. Popov, "Integral Method for Gratings," ch.4 *of Gratings: Theory and Numeric Applications*, ed. E. Popov (Institut Fresnel, CNRS, AMU, 2012) 95
www.fresnel.fr/files/gratings/Chapter4.pdf

5. G. Demésy, F. Zolla, A. Nicolet, and B. Vial, "Finite Element Method," ch.5 of *Gratings: Theory and Numeric Applications*, ed. E. Popov (Institut Fresnel, CNRS, AMU, 2012) 153
www.fresnel.fr/files/gratings/Chapter5.pdf

6. B. Stout, "Spherical harmonic Lattice Sums for Gratings," ch.6 of *Gratings: Theory and Numeric Applications*, ed. E. Popov (Institut Fresnel, CNRS, AMU, 2012) 203
www.fresnel.fr/files/gratings/Chapter6.pdf

7. E. Popov, "Differential Theory of Periodic Structures," ch.7 of *Gratings: Theory and Numeric Applications*, ed. E. Popov (Institut Fresnel, CNRS, AMU, 2012) 247
www.fresnel.fr/files/gratings/Chapter7.pdf

8. G. Granet, "Coordinate Transformation Methods," ch.8 of *Gratings: Theory and Numeric Applications*, ed. E. Popov (Institut Fresnel, CNRS, AMU, 2012) 301
www.fresnel.fr/files/gratings/Chapter8.pdf

9. F. Baida and A. Belkhir, "Finite Difference Time Domain Method For Grating Structures," ch.9 of *Gratings: Theory and Numeric Applications*, ed. E. Popov (Institut Fresnel, CNRS, AMU, 2012) 333
www.fresnel.fr/files/gratings/Chapter9.pdf

10. B. Gralak, "Exact Modal Methods," ch.10 of *Gratings: Theory and Numeric Applications*, ed. E. Popov (Institut Fresnel, CNRS, AMU, 2012) 371
www.fresnel.fr/files/gratings/Chapter10.pdf

11. S. Guenneau, R. Craster, Tr. Antonakakis, K. Cherednichenko, and Sh. Cooper, "Homogenization Techniques for Periodic Structures," ch.11 of *Gratings: Theory and Numeric Applications*, ed. E. Popov (Institut Fresnel, CNRS, AMU, 2012) 395
www.fresnel.fr/files/gratings/Chapter11.pdf